FPU problem & KdV equation

Padova - October 13, 2008

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Historical foreword: motivations
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- **Unexpected result**: for the examined systems, time-averages of relevant quantities do not approach the expected value (w.r. to the supposed ergodic measure) within the integration time.

- The motivation of the study goes back to earlier analytical works of Poincaré and Fermi himself on the subject.
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- The KdV equation is proposed as approximating somehow the FPU dynamics
- *Soliton*-like structures are numerically observed and their interaction properties used to explain some features of the FPU dynamics
- Two years later Kruskal and co-workers “solve” the KdV eqn by an Inverse Scattering technique, the first example of Lax-integrable PDE.
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- Kadomtsev-Petviashvili (KP): $(u_t + uu_x + u_{xxx})_x + u_{yy} = 0$
Study the \textit{prototype} Hamiltonian problem

\[
H_N(q, p) = \sum_{j=0}^{N-1} \left[ \frac{p_j^2}{2} + \frac{(q_{j+1} - q_j)^2}{2} + \alpha \frac{(q_{j+1} - q_j)^3}{3} \right]
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q_j(0) = \sum_{k=1}^{M_0} A_k \varphi_k(j), \quad p_j(0) = \sum_{k=1}^{M_0} B_k \varphi_k(j)
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\[
M_0/N \ll 1 \quad ; \quad E_N = H_N(q(0), p(0)) = N\varepsilon
\]
STRATEGY
**Strategy**

\[ (q, p)_{FPU} \xrightarrow{\text{Perturbation theory}} (\xi, \xi^*)_{FPU} \]

analyticity $\downarrow$

\[ U_{KdV} \xleftarrow{\text{reconstruction}} (u, u^*)_{FG-KdV} \]

Normal form $\uparrow$

\[ \xi, \xi^* \]
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\[\omega_k = 2 \sin \left(\frac{\pi k}{2N}\right)\]  

(dispersion relation)
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\[ k = 1, \ldots, N - 1 \]
\[ H_N(z, z^*) = \sum_{k=1}^{N-1} \omega_k |z_k|^2 + \frac{2\alpha}{3\sqrt{N}} \sum_{k_1, k_2, k_3=1}^{N-1} \Delta_{k_1,k_2,k_3} \prod_{s=1}^{3} \sqrt{\omega_{k_s}} \text{Re}(z_{k_s}) \]
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- the system eventually relaxes to equilibrium, characterized by modal energy equipartition: \( E_1 = \cdots = E_{N-1} \simeq \varepsilon \);
- a **metastable state**, or “quasi-state” characterized by an exponentially decaying energy spectrum -
  \( E_k \sim C \left( \frac{k}{N} \right)^\rho e^{-\gamma(\varepsilon)k/N} \) - persists for very long times.
INITIAL DATA:

\[ z_k(0) = \frac{A_k \omega_k + iB_k}{\sqrt{2\omega_k}}, \quad E_k(0) = \frac{B_k^2 + \omega_k^2 A_k^2}{2} \]
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An interesting example:

\[ z_k(0) = \sqrt{\frac{N\varepsilon}{M_0 \omega_k}} e^{-i\phi_k}, \quad E_k(0) = \frac{N\varepsilon}{M_0} \]

\((k = 1, \ldots, M_0, \text{zero otherwise})\) with different choices of the phases \(\phi_k\).
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One can plot the (normalized) modal energy spectrum: \[ E_k(t)/\epsilon \text{ vs. } k/N \] at different times.
Figure: Typical modal energy spectrum; $N = 1024$, $\varepsilon = 2.5 \cdot 10^{-4}$, 10% of modes initially excited [BLP08]
The effective number $M(t)$ of active modes at time $t$ is measured by a Boltzmann-Shannon-like counter:

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\mathcal{P}_k = \frac{E_k(t)}{\sum_h E_h(t)} = \frac{\omega_k |z_k(t)|^2}{\sum_h \omega_h |z_h(t)|^2}
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Effective density $f(t)$ of active modes:

\[
f(t) = \frac{M(t)}{N} = \frac{e^{S(t)}}{N}
\]

$\mathcal{P}_k = 1/N$ at equilibrium, and $f_{eq} = 1$. 

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**Figure:** Effective density \( f = M/N \) of active modes; \( N = 1024 \), \( \varepsilon = 2.5 \cdot 10^{-4} \) and \( 10^{-3} \), \( M/N = 0.1 \) initially [BLP08]
Mode-coupling is ruled by the selector

$$\Delta_{k_1,k_2,k_3} = \delta_{k_1+k_2,k_3} + \delta_{k_2+k_3,k_1} + \delta_{k_3+k_1,k_2} - \delta_{k_1+k_2+k_3,2N}$$

with corresponding processes

small denominators: forbidden to low modes

$$\omega_{k_1} + \omega_{k_2} \simeq \omega_{k_3=k_1+k_2}$$
Perform the canonical rescaling \((z, t, H_N) \mapsto (\zeta, \tau, K_N)\) defined by

\[
\zeta_k = \frac{z_k}{N\sqrt{2\epsilon}}, \quad \tau = \frac{t}{2N}, \quad K_N = \frac{H_N}{N\epsilon}
\]
Rescaling

Perform the canonical rescaling \((z, t, H_N) \mapsto (\zeta, \tau, K_N)\) defined by

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where \(0 < \epsilon = \varepsilon + O(\varepsilon^{3/2})\). Define \(\mu = \alpha\sqrt{\epsilon}\), \(L = 2N\sqrt{\mu}\) (\(\alpha > 0\) w.l.g.) and expand \(\omega_k\).
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\[
K_N(\zeta, \zeta^*) = \sum_{k=1}^{N-1} (2\pi k)|\zeta_k|^2 + \mu W(\zeta, \zeta^*) + O(\mu^2)
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\]

where

\[
W = -\sum_{k=1}^{N-1} \frac{(2\pi k)^3}{24L^2} |\zeta_k|^2 + \frac{2}{3} \sum_{k_1, k_2, k_3=1}^{N-1} \Delta_{k_1, k_2, k_3} \prod_{s=1}^{3} \sqrt{2\pi k_s} \text{Re}(\zeta_{k_s})
\]
Unperturbed ($\mu = 0$) motion: $\zeta = e^{-i2\pi J\tau} \zeta(0)$, 1-periodic in time, $J = \text{diag}(1, \ldots, N - 1)$ (i.e. $\zeta_k = e^{-i2\pi k\tau} \zeta_k(0)$).
Normalization

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Proposition (Averaging)

There exists a canonical transformation $(\zeta, \zeta^*) \mapsto (\xi, \xi^*)$, $\mu$-close to the identity, such that

$$K_N(\xi, \xi^*) = \sum_{k=1}^{N-1} (2\pi k)|\xi_k|^2 + \mu \overline{W}(\xi, \xi^*) + O(\mu^2)$$

where

$$\overline{W}(\xi, \xi^*) = \int_0^1 W(e^{-i2\pi J \tau} \xi, e^{i2\pi J \tau} \xi^*) \, d\tau$$
Introducing the time-dependent transformation to noncanonical co-rotating coordinates

$$(\xi, \tau, K_N) \mapsto (u, T, \overline{W} + O(\mu))$$

$$u = \sqrt{2\pi J} \ e^{i2\pi J \tau} \xi, \quad T = \mu \tau$$
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the resonant normal form Hamiltonian of the FPU system is

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\bar{W}(u, u^*) = -\sum_{k=1}^{N-1} \frac{(2\pi k)^2}{24L^2} |u_k|^2 + \frac{1}{4} \sum_{k_1, k_2, k_3=1}^{N-1} \delta_{k_1+k_2+k_3}(u_{k_1}^* u_{k_2}^* u_{k_3} + c.c.)
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up to a remainder \(O(\mu)\).
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\[
\frac{du_k}{dT} = -i(2\pi k) \frac{\partial \overline{W}}{\partial u_k^*}
\]
Truncated KdV as resonant normal form

Proposition

The Hamilton equations of $W(u, u^*)$ coincide with the Fourier-Galerkin truncation to the first $N-1$ modes of the KdV equation

$$U_T = \frac{1}{24L^2} U_{XXX} + \frac{1}{2} UU_X, \quad X \in \mathbb{T}(=\mathbb{R}/\mathbb{Z})$$

on the leaf: $\int_0^1 U \, dX = 0, \int_0^1 U^2 \, dX = 2$.

Thus the KdV equation in the small dispersion regime ($L \propto N\epsilon^{1/4}$ very large) describes the dynamics of the FPU problem on the time-scale $t \sim N/\sqrt{\epsilon}$ (recall that $T = t\sqrt{\epsilon}/N$).
The Fourier-Galerkin projection operator $P^N$ is defined by

$$(P^N U)(X, T) = \sum_{k=-N+1}^{N-1} \hat{U}_k(T) e^{-i2\pi kX}.$$
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One has

$$\overline{W} = -\frac{1}{48L^2} \int_0^1 (u^N_X)^2 dX + \frac{1}{12} \int_0^1 (u^N)^3 dX$$
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and

\[
\frac{d u_k}{dT} = -i(2\pi k) \frac{\partial \overline{W}}{\partial u_k^*} \iff u^N_T = \partial_X P^N \left( \frac{\delta \overline{W}}{\delta u^N} \right)
\]
Recall that $U_T = \frac{1}{24L^2} U_{XXX} + \frac{1}{2} UU_X$ and $L \propto N\varepsilon^{1/4}$, $T \propto \sqrt{\varepsilon t}/N$. 
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\epsilon \rightarrow \lambda \epsilon \quad , \quad N \rightarrow \lambda^{-1/4} N \quad , \quad t \rightarrow \lambda^{-3/4} t
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leaves the KdV equation invariant. Based on Cauchy estimates, for the effective density of active modes \( f = M/N \) one expects

\[
f \propto \frac{L}{N} = \epsilon^{1/4} \quad \Rightarrow \quad f \rightarrow \lambda^{1/4} f
\]

This is checked numerically:
Figure: From left to right: KdV rescaling [BLP08]
Theorem (Kappeler-Pöschel 07)

Consider the KdV equation $U_T = \delta U_{XXX} + \frac{1}{2}UU_X$.

If the initial datum $U(X,0)$, $X \in \mathbb{T}$, is analytic in the (maximal) complex strip $\{|\text{Im}(z)| \leq a\}$, then there exists $0 < \rho(\delta) \leq 1$ s.t. the corresponding solution $U(X, T)$ is analytic in the complex strip $\{|\text{Im}(z)| \leq a\rho(\delta)\}$ for any $T \in \mathbb{R}$. 
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That is to say: analytic initial data evolve into global solutions which are analytic in a possibly narrower but finite-width strip.
Regularity of KdV solutions

**Theorem (Kappeler-Pöschel 07)**

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That is to say: analytic initial data evolve into global solutions which are analytic in a possibly narrower but finite-width strip. No estimate of \( \rho(\delta) \) available: we are interested in the limit \( \delta \to 0 \)!
Consider the KdV equation $U_T = \frac{1}{24L^2} U_{XXX} + \frac{1}{2} U U_X$. 
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By the TKP thm, \( U(z, T) \) analytic in \( \{ |\text{Im}(z)| \leq \sigma(T; L) \} \).
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\mathcal{M}(T; L) \equiv \max_{\text{Re}(z) \in [0, 1], |\text{Im}(z)| = \sigma(T; L)} |U(z, T)|
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Notice that as $L \to \infty$ the KdV eqn approaches the Burgers-Hopf eqn $U_T = \frac{1}{2} U U_X$, whose solutions display vertical slopes in a finite critical time $T_c = O(1)$.
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\sigma(T; L) \sim \frac{c(T)}{L} \quad (L \to \infty)
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$U(X, T)$: solution of the KdV eqn with in.dat. $U(X, 0)$;
Asymptotic reconstruction

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**Theorem (Kalisch 05)**

Suppose $U(X, 0) \in \mathcal{H}^{a_0, s}$, where $a_0 > 0$ and $s > 0$; then, for any fixed $T > 0$ there exist two positive constants $\lambda(T)$ and $a(T)$ s.t.

$$\sup_{t \in [0, T]} \| U(\cdot, t) - u^N(\cdot, t) \|_{L^2} \leq \lambda(T) \frac{e^{-a(T)N}}{N^{s-1}}$$
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That is to say: $u^N$ and $U$ can be made arbitrarily close on any fixed time-interval if $N$ is large enough.
Conclusions: open problems

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- Extension to other models, in particular to the quartic one leading to the mKdV eqn: a very few results available!
- Second stage of the story: breakdown of KdV approximation and estimate of the time-scale to equipartition.